Overview: Distribution Estimation, MEMS Optimization, and Disease Modeling

Brian M. Adams

Optimization and Uncertainty Estimation (Org. 1411)

Center 1400 LTE Review (Sep. 2005 – Jan. 2006)

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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Overview

- Introduction and research interests
  - Academic background
  - Nonparametric distribution estimation
- Initial SNL projects and impact
  - Large-scale disease model for bioagent detection
  - Reliability-based shape optimization for MEMS
  - DAKOTA/UQ analysis for QASPR project
  - DAKOTA interfaces / capabilities
- Anticipated professional activity

Brian M. Adams

- LTE in 1411 since 09/19/2005
- Ph.D. in Computational and Applied Mathematics (w/ H.T. Banks), North Carolina State University
- Dissertation on nonparametric parameter identification (inverse) problems in HIV infection
- Collaborated on optimal control of HIV via treatment interruptions

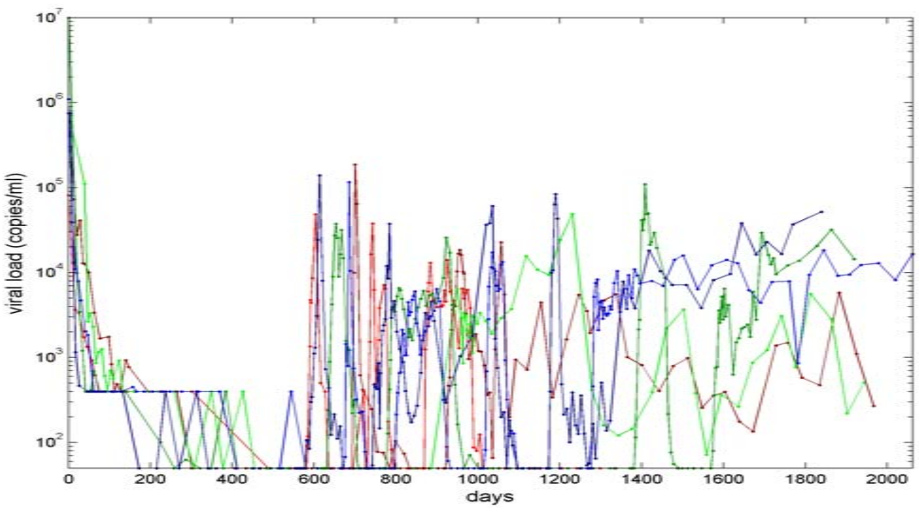
Research Interests

Integration of science, mathematics, computation:

- Parameter estimation, theory and methods for estimation of uncertain parameter *distributions*
- Modeling infectious disease, complex biological systems, including agent-based modeling
- Optimization technology and software
- Reduced-order models, especially in non-traditional (complex systems) settings
- Scientific computing and software development

Nonparametric Distribution Estimation

HIV viral load data *y(t)* for 6 patients



Biologically-based dynamics model (for *each* patient *j*)

$$\dot{x}(t) = g(t, x; \vec{q}^{\,j})$$

$$y^j(t) = x(t; \vec{q}^{\,j}) + \varepsilon^j(t, x)$$

- **Assume each patient has parameter vector** q^j**, so** q^j ***distributed across population***
- **Would a particular distribution of parameters** q **explain long-term inter-patient variability?**
- **Given only outputs** $y^j(t)$ **and the DE model, identify the probability density function** $f(q)$ **for parameters** q **that gave rise to them (an *inverse problem* to determine** $f(q)$**)**

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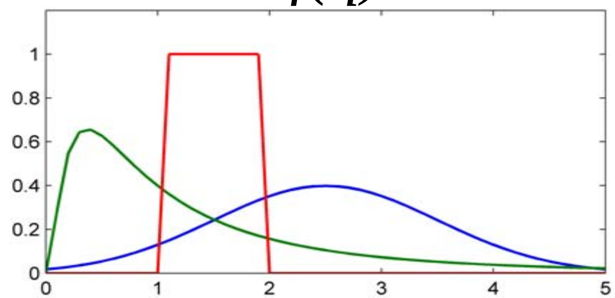
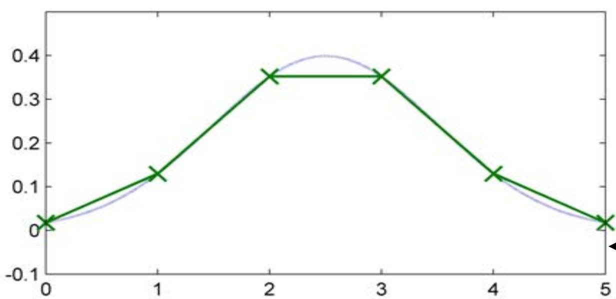
Estimating Distributions from Data

f(q)





Simple cost criterion can distinguish between distributions…

$$\min_f J(f) = \sum_{i,j} \left| E\left[x(t^i; q) \mid f(q) \right] - y^{ij} \right|^2$$

$$= \sum_{i,j} \left| \int x(t^i; q) f(q) dq - y^{ij} \right|^2$$

Computationally: pick basis and optimize over coefficients

- **How to best parameterize densities? How to measure fit?**
- **General theory for inversion in this context**
- **How sensitive are model outputs to distribution? Derivatives with respect to probability measures (active research area)**

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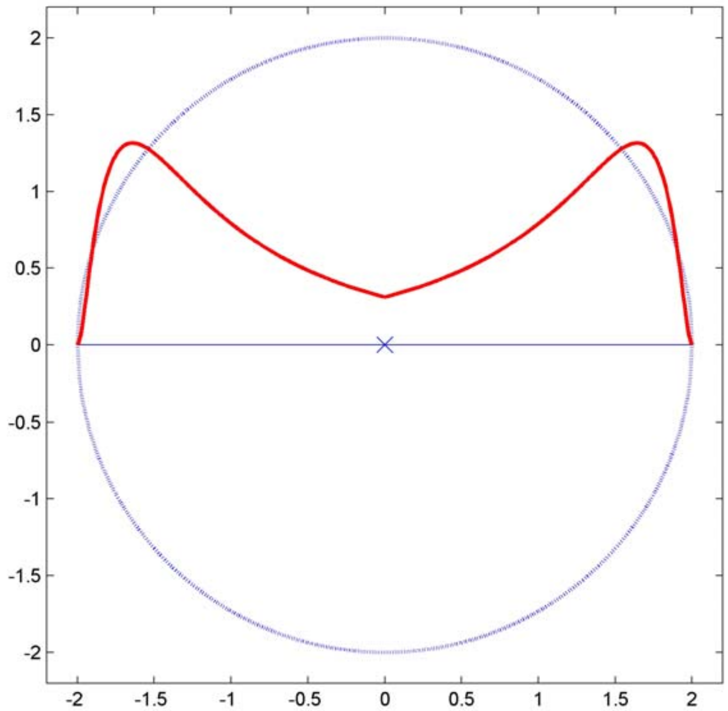
Potential Application to MEMS

- **Micro-Electro Mechanical Systems manufacturing**
  - **Highly variable output: devices vary substantially across wafer, fabrication runs**
  - **Yield problems: serviceable device yield often extremely low**
- **Given distribution of finished products and process model, invert to understand (via distributions) inputs to or events during process**



…edge bias varies across wafer?

Potential implementation as new DAKOTA feature

Large-scale Disease Model

GOAL: Identify location and time of insertion of bioterror agent in a community

- **1st year of LDRD with Jaideep Ray (8964) and Karen Devine (1412)**
- **Large-scale agent-based model to simulate spread of disease: millions of people, thousands of locations they might visit.**
- **Based on presentation at clinics with symptoms – assume sensors did not detect**
- **Use Bayesian techniques for the inverse (source identification) problem, given clinical presenters**

Contributions to Disease Model

- **Develop efficient disease propagation model for smallpox, anthrax, etc.**
  - **Leverage my background in biological systems modeling and coursework in epidemic modeling to build biologically-based model**
  - **Determine efficient scheme for computing given bipartite person/location graph with millions of nodes – *possibly implement in Trilinos framework.* Parallel scaling important.**
  - **Develop network or matrix sampling methods to create Reduced Order Model – only need sufficient resolution for inverse problem. Reduced case should be laptop-friendly.**

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computationally
multi-scale

RBDO for MEMS

- MESA-centered projects for Reliability-Based Design Optimization of Micro-electro mechanical systems (MEMS) using quantified uncertainty
- Bistable MEMS mechanism:
  target for ASC Level II milestone for error-corrected reliability analysis of MEMS
  - Working with on error corrected reliability for MEMS *(with Mike Eldred, Kevin Copps, Pat Notz, Jon Wittwer)*
  - Idea: use directional error estimates on quantities of interest from finite element codes (SIERRA: Andante, Aria) to improve and bound reliability predictions in DAKOTA

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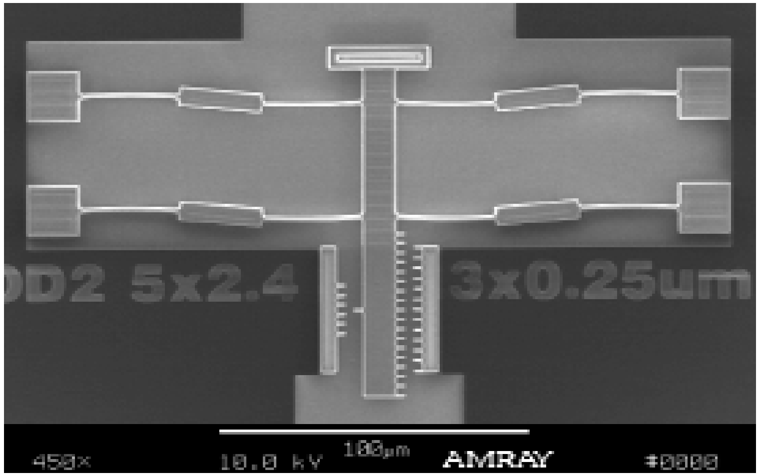
RBDO: Bistable MEMS Mechanism

- **Bistable device: switch, relay, nonvolatile memory**
- **Typical manufacturing uncertainties:**
  - **Width and length of in-plane features (due to photo mask)**
  - **Thickness of silicon layers**
  - **Young's modulus, residual stress**
- **Interfaced DAKOTA/UQ with SIERRA Adagio code for solid mechanics analysis**
- **Performed geometric shape optimization**



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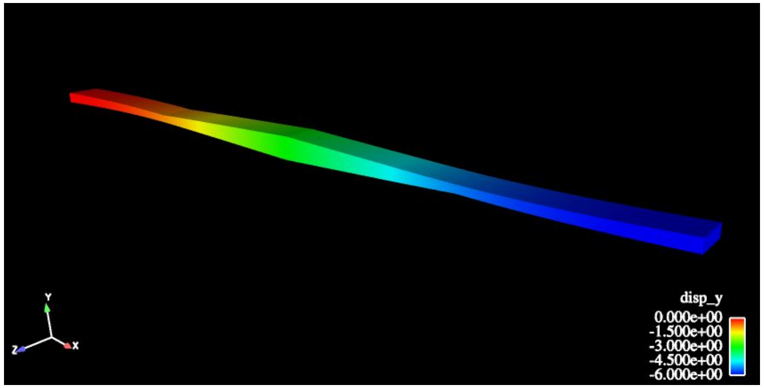
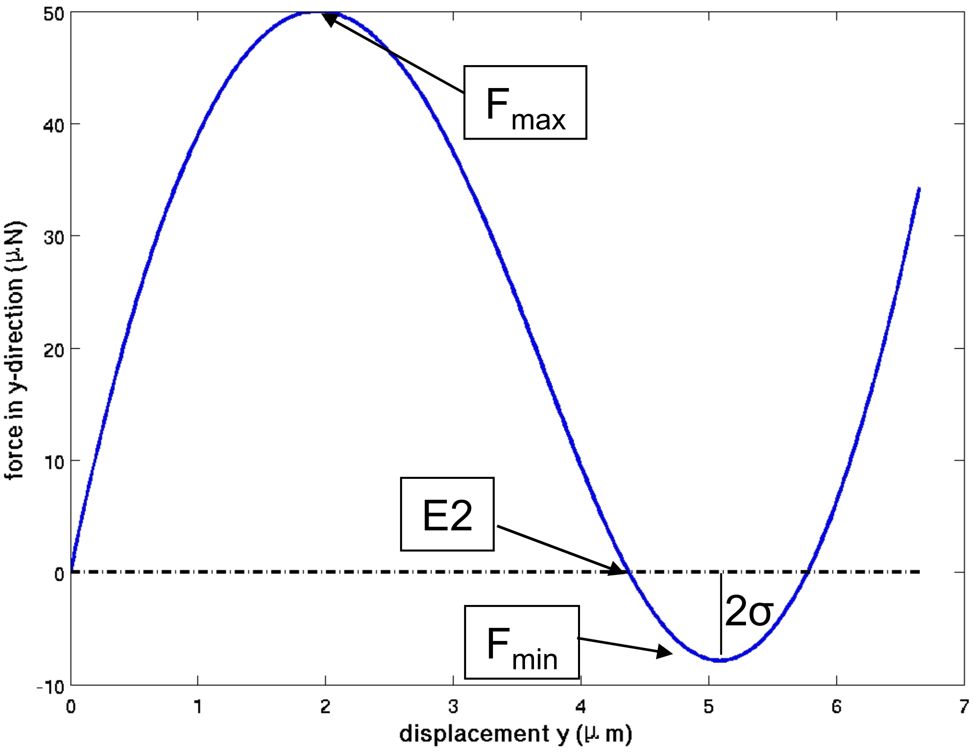


with Mike Eldred (1411), Jon Wittwer (1769), others

RBDO: Bistable MEMS Mechanism

- **Objective: Given uncertainty, reliably maintain bistability ($F_{min} < 0$) while minimizing actuation force (drive F_{min} to 0)**
- **Define failure to be $F_{min} > 0$ and perform reliability-constrained optimization**

$$\max_{d} F_{\min}(d)$$
$$s.t.\ 2 \le \beta(d)$$
$$50 \le F_{\max}(d) \le 150$$
$$E2(d) \le 8$$



Opportunity for DAKOTA designs to impact fabrication in Feb. 2006

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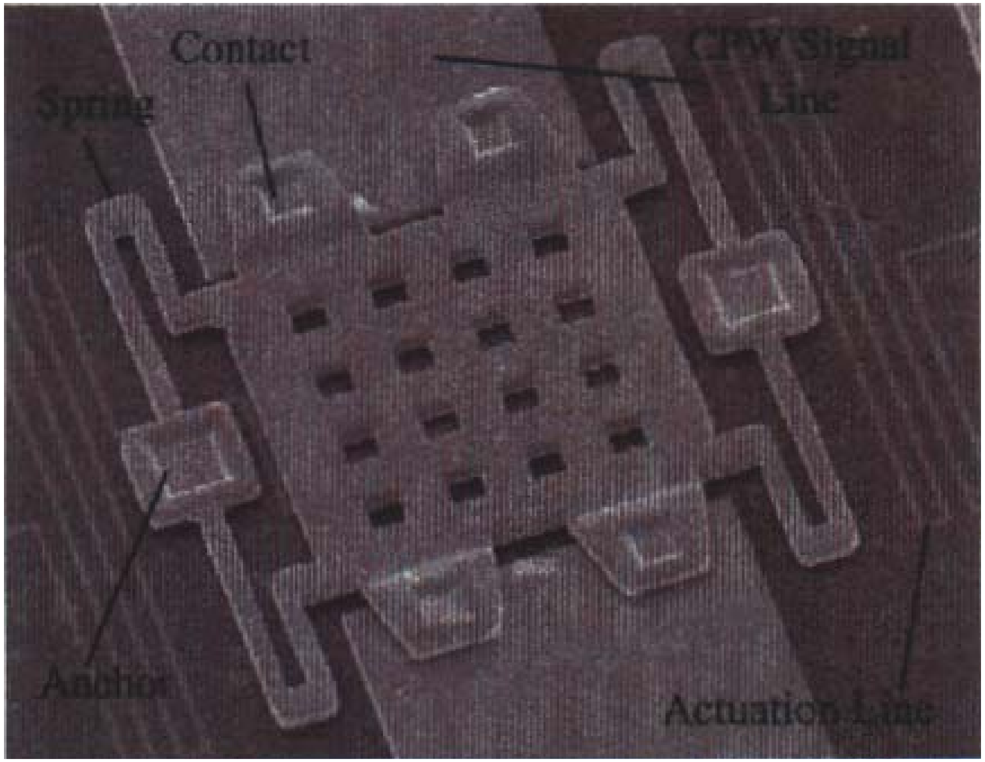
RBDO: MESA RF Ohmic Switch

- **Applying DAKOTA to optimize waveform for current best design (with Jordan Massad and Rich Field, 1524)**
- **Complete redesign (concept and geometry – Steve Thomas, 1411) to eliminate vibrations, improve reliability**
- **Performing shape optimization for existing and new design**
- **Satellite and synthetic aperture radar (SAR) applications.**



current design (*Dyck (1742), et. al., SAND2003-2210A*)

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QASPR: Uncertainty Quantification

- Rapidly interfaced DAKOTA to research Fortran code for analyzing defects in silicon
- Demonstrated UQ software advantage over manual single-parameter sensitivity analyses
- Showed correlation of uncertain input variables to current at several output times in simulation
- Impact: important proof of concept for further QASPR UQ studies employing Charon, Xyce
- Collaborators: Tony Giunta (1533), Bill Wampler (1111), Sam Myers (1112)

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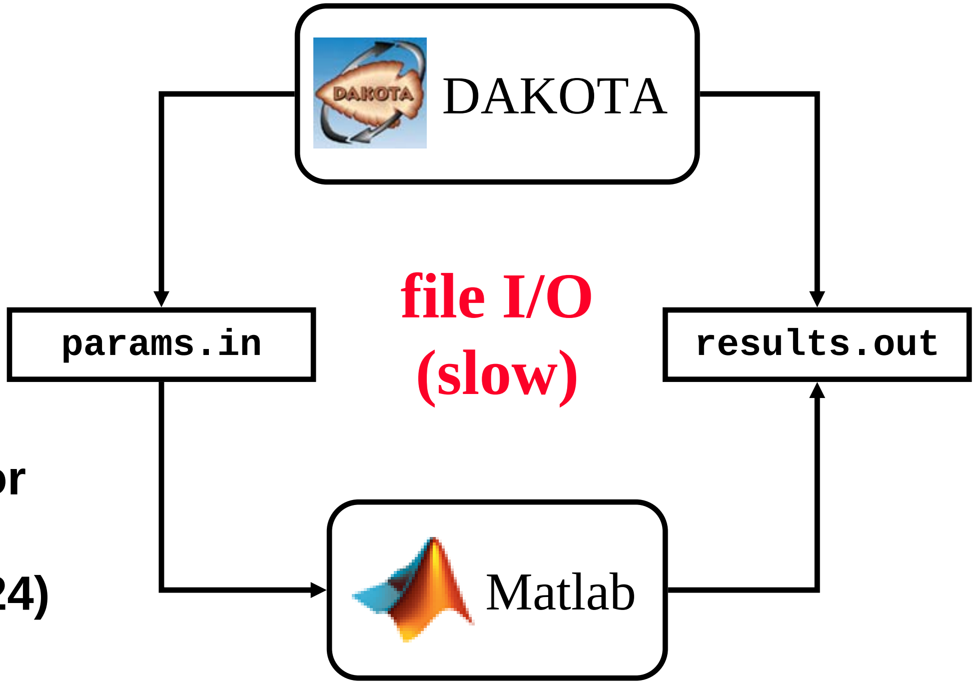
DAKOTA Interfaces/Capabilities

- **User-requested DAKOTA-Matlab *close-coupled, efficient* interface**
  - **Enables convenient use of Matlab-based simulations with DAKOTA**
  - **Impact: optimized diffraction gratings (Louis Romero, 1414);**
  - **Impact: waveform optimization for MEMS RF switch (Rich Field & Jordan Massad, 1524)**



- **Generated DAKOTA-Mathematica black box interface example, close-coupled in progress (with Shane Brown, 1411)**
- **Implementing automatic variable and constraint scaling (LM SV requirement)**

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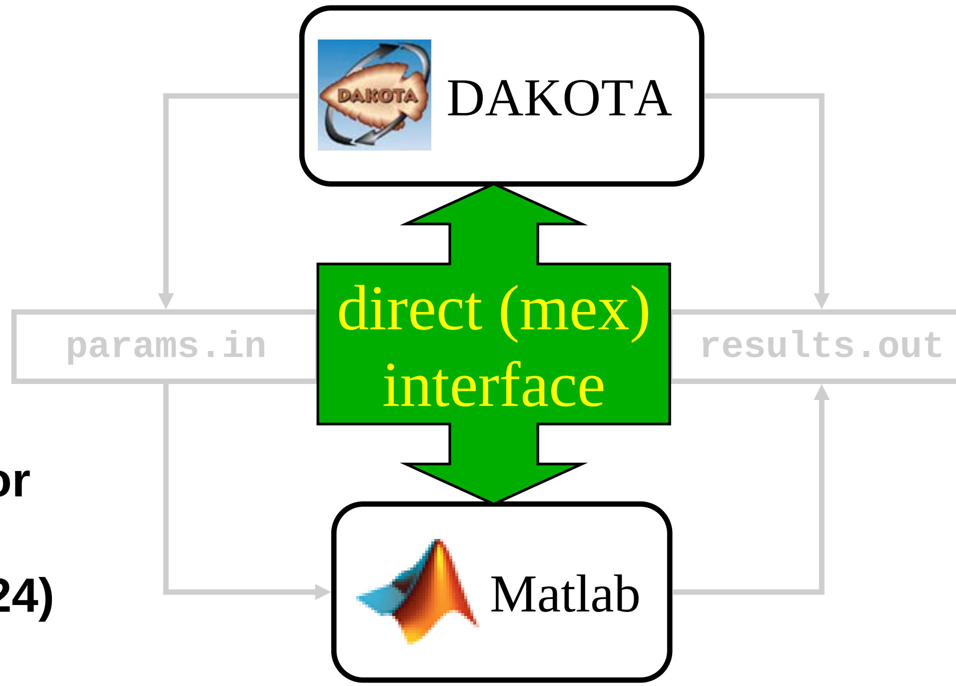

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Professional Activities

Publications

- ***Model fitting and prediction with HIV treatment interruption data*** **(submitted Sept. 2005)**
- **Two conference proceedings papers on *RBDO for MEMS* in progress with Mike Eldred (REC, AIAA)**

Conferences / courses

- **Invited lecture at Mathematical Biosciences Institute, Spring 2006**
- ***Epidemiology and Public Health*** **mini-symposium invited speaker, SIAM Annual Meeting, July 2006**
- **Attend Copper Mountain Conference on Iterative Methods, other optimization, design conferences**
- **SNL Lunchtime MEMS design short course series, Spring 2006**

Service

- **Co-mentor summer C.S. student from UIUC (with Karen Devine)**